CHEMICAL PHYSICS

Volume 178, number 1,2,3, 15 December 1993

Contents

Numerical application of the coupled cluster theory with localized orbitals to polymers. I. Total correlation energy per unit cell YJ. Ye, W. Förner and J. Ladik	1
An investigation of the outermost orbital momentum distributions of formaldehyde, acetaldehyde and acetone, by electron momentum spectroscopy and quantum chemical calculations at the SCF and MRSD-CI levels	
B.P. Hollebone, P. Duffy, C.E. Brion, Y. Wang and E.R. Davidson	25
Theoretical investigations of the electronic spectra of ZnCH ₃ . Analysis of spin-orbit coupling and Jahn-Teller effect	
Ch. Jamorski, A. Dargelos, Ch. Teichteil and J.P. Daudey	39
The Green function method in the theory of nuclear and electron spin polarization. I. General theory, zero approximation and applications	4.77
P.A. Purtov and A.B. Doktorov	47
Disordered polaron transport: a theoretical description of the motion of photoinjected charges in molecularly doped polymers D.H. Dunlap and V.M. Kenkre	67
On the relative stabilities of the linear and triangular forms of B ₃ N Z. Slanina, J.M.L. Martin, JP. François and R. Gijbels	77
Density dependent structural properties of dilute mixtures of OCS with argon. A molecular dynamics investigation J. Samios, D. Dellis and H. Stassen	83
Molecular dynamics simulation of the plastic phase of 2-methyl-2-nitropropane S. Labate, G. Cardini, R. Righini and S. Califano	93
Thermodynamic perturbation theory of charged hard spheres in a uniform neutralizing background	
J.W. Lee, M.S. Jhon and F.H. Ree	105
Forward and reverse excitation energy transport and concentration depolarization in two- component systems L. Kułak and C. Bojarski	113
Scaled ab initio force field of E- and Z-hexatriene in the S ₀ and T ₁ states	- 10
F. Negri, G. Orlandi, F. Zerbetto, P. Palmieri and R. Tarroni	133
Sum rules for atomic polar and axial tensors from vibronic coupling theory D. Yang and A. Rauk	147

(continued on page 3 of cover)



0301-0104(19931215)178:1/3:1-L

Contents

(continued from page 4 of cover)

Potential energy surfaces of ozone in its ground state and in the lowest-lying eight excited states A. Banichevich, S.D. Peyerimhoff and F. Grein	155
The rovibrational ν_2 Raman spectrum of ammonia: a comparison of theory and experiment P.E.S. Wormer, E.H.T. Olthof, R.A.H. Engeln and J. Reuss	189
Valence electronic structure of a long-chain alkane in random-coil forms. Gas-phase UPS of n-C ₃₆ H ₇₄ and MO calculations K. Seki, N. Sato and H. Inokuchi	207
Theoretical studies of the electronic spectrum of SiF ₂ ZL. Cai and JL. Bai	215
Ro-vibronic spectrum of the N_2O^+ ion in the X $^2\Pi$ state H. Gritli, Z.B. Lakhdar, G. Chambaud and P. Rosmus	223
Effective core potential study of transition metal and lanthanide catalyzed hydrogen exchange T.R. Cundari, W.J. Stevens and S.O. Sommerer	235
Theoretical calculations of the quartet potential energy surfaces in the $NH^+ + H_2$ system R. Polák, I. Paidarová and P.J. Kuntz	245
Are there geometric isomers of the van der Waals dimers Ar-OCS and Ar-SO ₂ ? R.G.A. Bone	255
Theoretical study of the lowest potential energy surfaces for the reaction $O(^3P) + HBr(X\ ^1\Sigma^+) \rightarrow OH(X\ ^2\Pi) + Br(^2P)$ J. Urban and V. Staemmler	279
A quasiclassical trajectory study of the effect of the initial rovibrational level and relative translational energy of reactants on the dynamics of the $N(^4S_u) + O_2(X\ ^3\Sigma_g^-) \rightarrow NO(X\ ^2\Pi) + O(^3P_g)$ atmospheric reaction on the $^2A'$ ground potential energy surface M. Gilibert, A. Aguilar, M. González and R. Sayós	287
A matrix isolation study of the inter- and intramolecular vibrations of the water-acetone complex A. Engdahl	305
Statistical simulation of IF angle and angle–velocity distributions from the crossed beam reaction $F+I_2\!\to\! IF+I$	
PA. Elofson and L. Holmlid	315
A detailed SACM study of the H+NO→HNO reaction based on a realistic potential energy surface C.J. Cobos	329
Zeeman effect in T _{1u} symmetry vibrational states of C ₆₀ fullerene M. Pawlikowski, M. Pilch and T.A. Keiderling	341
Splitting of the 1s ⁻¹ 3p resonance in sulfur K XANES by surroundings in compounds with sulfur- carbon double bond	
KH. Hallmeier, A.A. Pavlychev, R. Szargan, L. Beyer, C. Hennig and F. Thiel	349
Ground- and lowest excited-state MRDCI potential-energy surfaces for the collinear Li+HF	
reaction C. Suárez, A. Aguado and M. Paniagua	357
(continued on preced	ing page)

Contents

Vibrational exchange in the manifold of high-frequency vibrations of the CH ₂ F ₂ molecule P.I. Ionov, A.A. Kosterev, A.L. Malinovsky and E.A. Ryabov	363
Structural relaxation in amorphous biphenyl and a new crystalline phase H. Nakayama, M. Kawahara and K. Ishii	371
Laser excitation and emission spectroscopy of the methoxy radical in a supersonic jet P. Misra, X. Zhu, CY. Hsueh and J.B. Halpern	377
The electronic spectrum of water in the discrete and continuum regions. Absolute optical oscillator strengths for photoabsorption (6-200 eV) W.F. Chan, G. Cooper and C.E. Brion	387
The electronic spectrum of carbon dioxide. Discrete and continuum photoabsorption oscillator strengths (6-203 eV) W.F. Chan, G. Cooper and C.E. Brion	401
Time resolution of ion pair formation in poly (N-vinylcarbazole) S. Nešpúrek	415
Fluorescence lifetime measurements and hole-burning experiments on J-aggregates of a benzimidocarbocyanine dye M. Lindrum, A. Glismann, J. Moll and S. Daehne	423
Measurement of very long (10 ⁷ s) spin conversion times: dimethyl-s-tetrazine in durene M. Joyeux, B. Prass, C. von Borczyskowski, JC. Vial and H.P. Trommsdorff	433
Optical properties of a streptocyanine dye single crystal with tubelike aggregation: bis(dimethylamino)-heptamethinium tetrafluoroborate BDH+BF ₄ -L. Dähne, A. Horvath and G. Weiser	449
The electronic absorption spectra and bonding of cobalt(II) doped into the low-symmetry hosts, KCdCl ₃ and KCdBr ₃ R.G. McDonald, A.A. Al-Waili and W.E. Smith	459
Absorption and emission spectra of C ₆ F ₅ X ⁺⁻ (X=H, F, Cl, Br, and I) radical cation in perfluorohexane matrix T. Oomori and T. Hikida	477
Normal modes of 4-aminobenzonitrile (4-ABN). A comparison of PM3 calculations with experimental jet-cooled spectroscopy H. Yu, E. Joslin, S.M. Zain, H. Rzepa and D. Phillips	483
Excited-state intramolecular proton transfer in jet-cooled 1-hydroxy-2-acetonaphthone A. Douhal, F. Lahmani and A. Zehnacker-Rentien	493
Study of isotope effects in the ground state of the symmetrical isotopomers of CuCl ₂ P. Crozet, J.C. Coste, R. Bacis, A.J. Bouvier, S. Churassy and A.J. Ross	505
Reveal of local symmetry of electron-vibration interactions in fine-structure fluorescence spectra of complex molecules. Amino- and hydroxy-tetrasubstituted anthraquinones E.A. Gastilovich and K.V. Mikhailova	515
Characterization of Tl-rare gas complexes and comparison with other group 3A metal complexes A. Stangassinger, J. Scheuchenpflug, T. Prinz and V.E. Bondybey	533
(continued on preced	ling page)

Contents

Time-resolved LIF spectroscopy on N ₂ (A) metastable in a He/N ₂ pulsed rf discharge S. De Benedictis, G. Dilecce and M. Simek	547
Radiative lifetimes of the A $^2\Sigma_{1/2}^+$ and $X_2^2\Pi_{3/2}$ states of lead monohalides O. Shestakov, H. Demes and E.H. Fink	561
A 2+1 REMPI study of the E-X transition in CO. Indirect predissociations in the E ¹ Π state J. Baker, J.L. Lemaire, S. Couris, A. Vient, D. Malmasson and F. Rostas	569
Singlet state energy levels of $C_2H_4^{2+}$ by double charge transfer spectroscopy P.G. Fournier, J. Fournier, M.L. Langford and F.M. Harris	581
Small angle X-ray scattering and viscoelastic studies of the molecular shape and colloidal structure of bovine and rat serum albumins in aqueous systems T. Matsumoto and H. Inoue	591
Structural phase transitions and orientational ordering in C ₇₀ G.B.M. Vaughan, P.A. Heiney, D.E. Cox, J.E. Fischer, A.R. McGhie, A.L. Smith, R.M. Strongin, M.A. Cichy and A.B. Smith III	599
Erratum	615
Author index	616
Subject index	622
Instructions to authors	636

